

Electronic Structure of $\text{Sr}_2\text{FeMoO}_6$: X-ray Fluorescence Measurements

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Colossal magnetoresistance (CMR) has attracted much attention due to the importance of its potential technological applications as well as the unusual fundamental magnetic properties. During the last decade the interest concentrated on systems based on doped manganites. Their behaviour is well understood in terms of double-exchange mechanism. Most recently, a CMR effect in the ordered double perovskite $\text{Sr}_2\text{FeMoO}_6$ was reported [1]. This compound exhibits intrinsic tunnelling-type magnetoresistance at room temperature. Its structure and fairly high magnetic transition temperature (T_c) have been reported long time ago [2]. The latest investigations have concentrated on the theoretical description of the magnetic and electronic structure of this compound [3,4]. In contrast, experimental investigation dealing with the electronic structure are rare. We report the first SXF measurements done at the ALS Beamline 8.0.1, obtained on polycrystalline samples of $\text{Sr}_2\text{FeMoO}_6$.

The conduction and the valence band in $\text{Sr}_2\text{FeMoO}_6$ are known to consist of Fe 3d, O 2p and Mo 4d states. A big advantage of the SXF method is the symmetry-selective absorption-emission process. Starting at the Fe 2p core levels one can excite the electrons to the nd and ns levels due to the selection rules for optical transitions. According to band structure calculations, the Fe $L_{2,3}$ absorption and emission processes will show high intensity and direct conclusions can be drawn concerning the electronic structure.

In figure 1 the absorption and emission spectra at the Fe 2p threshold are displayed. Both spectra consist of two main structures which are due to the spin orbit splitting of the Fe 2p core level. The energy positions of the spectra lead to the conclusion that a metallic behaviour of the sample can be expected. Indeed, $\text{Sr}_2\text{FeMoO}_6$ shows a halfmetallic behaviour. The shape of the absorption spectra agrees well with the calculated density of empty states [1]

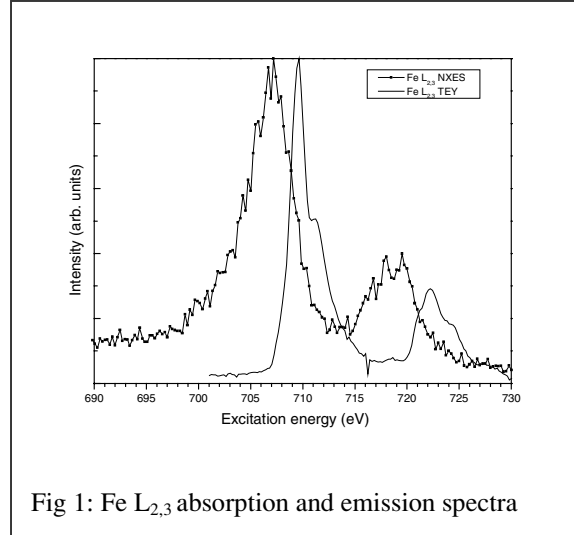
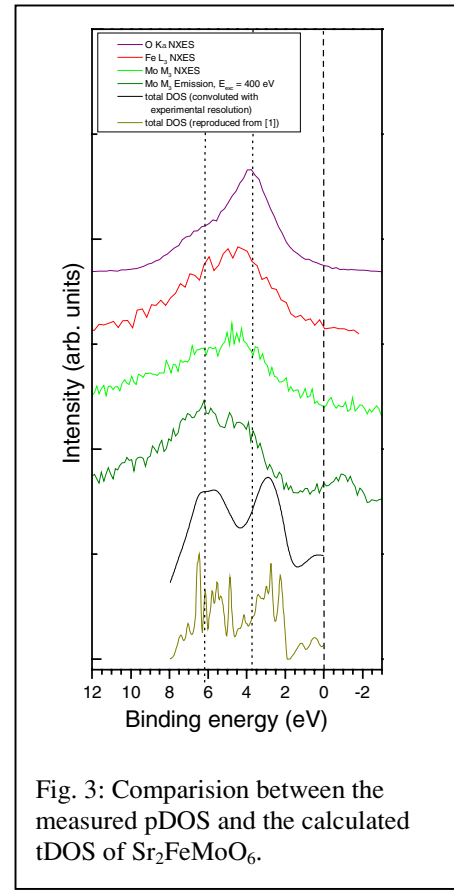
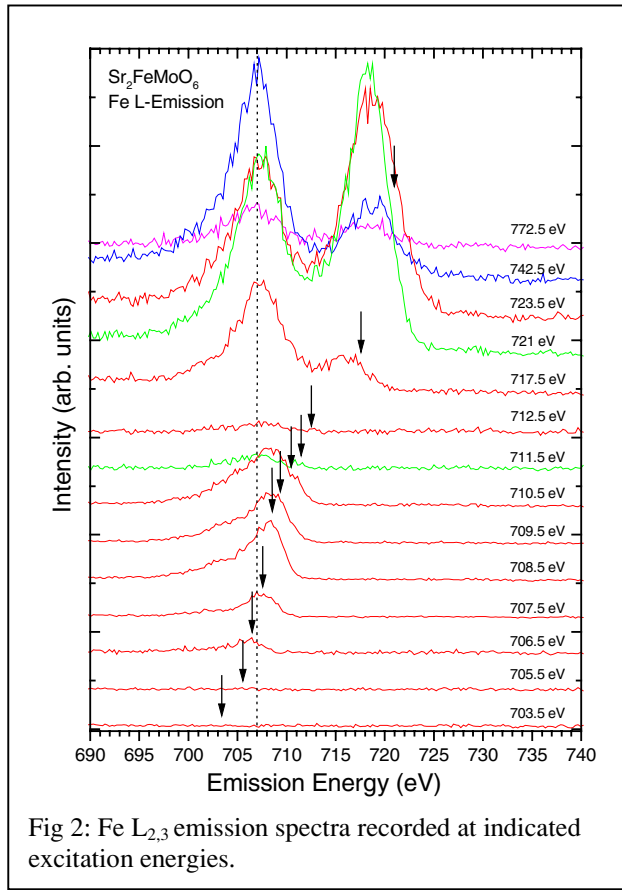


Figure 2 shows emission spectra at various excitation energies (reported by arrows). The Fe $L_{2,3}$ emission features are strongly dependent on the excitation energy. The dotted vertical line indicates the energy position at the normal emission (NXES) which can be observed at 707 eV. At excitation energies around the L_2 absorption threshold, an emission feature can be observed at 708.5 eV. Going



up with the excitation energy just above the absorption maximum (711.5 eV) the emission intensity drops nearly to zero. Reaching the Fe L_3 absorption with excitation energy (721 eV and 723.5 eV) a growing emission intensity can be observed. The L_2 emission now can be found at 707 eV, the main L_3 emission peak at about 719 eV. A strong resonance can be observed. At 772.5 eV excitation energy the normal x-ray emission takes place and at this energy the absorption and the emission processes can be assumed to be independent. At the L_3 resonance the emission energy doesn't shift to higher energy compared to the L_2 resonance. This leads to the conclusion that the emission spectra have to be interpreted by the spin dependent partial Fe 2p density of states modified by the specific transition probabilities. A detailed interpretation of the emission spectra in these terms will be done in the near future.

The partial density of states of the elements forming the valence band are shown in figure 3 together with the calculated total density of states (taken from [1]). The valence band consists mainly of two states, one at 3 – 4 eV, the other one at about 8 eV (note that the scale was converted to binding energy). All emission spectra reveal also a two peak structure, which indicates a strong hybridization between oxygen 2p and molybdenum 4d and iron 3d, respectively. Again, all spectra are in good agreement with the calculation. For Mo, also an emission spectrum, recorded at an excitation energy of 400 eV (just above the M_3 absorption threshold), is displayed. In this spectrum the peak at 8 eV shows a strong intensity compared to the NXES spectrum. This behavior could be due to the emission from the Mo 4d down spin state. The reason for this strong resonance is not completely clarified so far.

In conclusion it can be said that the emission spectra obtained on the Mo M_2 and Fe $L_{2,3}$ show a strong excitation energy dependance. For explanation a detailed analysis of the data and a comparison with calculation have to be done. The oxygen K_α spectra (not presented here) are only weakly depending on the excitation energy.

References

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